

The Development of a Framework for CFD Validation and Best Practice: The QNET-CFD Knowledge Base

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Abstract: QNET-CFD is a thematic network on quality and trust for the industrial applications of Computational Fluid Dynamics (CFD), developed under the European Union R&D program. The main objectives of QNET-CFD were to collect CFD and experimental data in a systematic and quality controlled way and to set the basis for a consistent Knowledge Base in support of CFD guidance and validation. The QNET-CFD activity was organized around six Thematic Areas (TAs) covering the following industry sectors: external aerodynamics; combustion & heat transfer; chemical process, thermal hydraulics and nuclear safety; civil construction & HVAC; environment; turbomachinery internal flows. The main outcome of the QNET-CFD actions is the Knowledge Base (KB) with contains in a user oriented interface, extensive experimental and CFD data for a large number of test cases subdivided into 53 Application Challenges (AC) and 43 Underlying Flow Regimes (UFR). The KB contains, in addition to state-of-the-art reviews for each of the six thematic areas, Best Practice Advice (BPA) in the use of CFD for most of AC. This is considered as a significant contribution from the QNET-CFD activities and it is expected that the level of the thrust and quality in CFD will hereby be improved.

Key words: QNET-CFD; CFD; thematic network; knowledge base

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摘 要: QNET-CFD 是欧盟 R&D 项目开发的一个主题网络,该网络讨论了计算流体力学(CFD)供工业应用应具有的品质和可信度,其主要目的是以系统和质量控制的方式收集 CFD 和实验数据,建立两者相容的知识库(KB),以此为基础,支持对 CFD 进行指导和评估。QNET-CFD 围绕覆盖下述工业部门的 6 个主题(TA)组成:外流空气动力学;燃烧和传热;化学过程、热力学和核安全;土木建筑和 HVAC; 环境; 涡轮机内流。其主要成果是建立了具有面向用户界面及丰富的实验和 CFD 数据的知识库,这些数据来自于大量实验数据,分为 53 种应用挑战(AC)和 43 种基本流动状态(UFR)。除对上述 6 个主题领域中每一个的科学动态给出述评外,KB 还包含了对大多数应用挑战如何利用 CFD 的最实际的建议,这被视为 QNET-CFD 最有意义的贡献,CFD 的可信度和质量水平将因此得以进一步提高。

关键词: QNET-CFD; 计算流体力学; 主题网络; 知识库

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With the strong development of CFD and the increasing complexity of the geometrical and physical conditions of current industrial CFD simulations, there is a growing need to establish generally recognized and accepted quality assurance criteria for evaluating the CFD results. This requirement is amplified by the needs of the virtual prototyping methodologies as applied in industry, whereby de-

sign decisions are increasingly based on simulation results. This applies to all areas of Computational Aided Engineering(CAE), and so much more to CFD, due to its complexity related to numerous uncertainties and error sources. The main sources are a combination of numerical errors, uncertainties in turbulence modelling, amplified by the nonlinear flow properties and by multidisciplinary physics,

such as fluid-structure, fluid-thermal interactions. QNET-CFD is a first systematic attempt towards these objectives, with a first objective of providing Best Practice Advices (BPA) for a variety of industrial relevant flow configurations. This paper presents the main organisational structure of this effort, its systematic approach and the resulting outcome under the form of a computerized Knowledge Base (KB).

1 Objectives and Organisation of QNET-CFD

The QNET-CFD initial development started from the Best Practice Guide for CFD generated by the Quality and Trust Special Interest Group (SIG) of ERCOFTAC (European Research Community on Flow Turbulence and Combustion), led by Dr. Anthony Hutton. This initiative of ERCOFTAC, involved European code developers, code vendors, academics and industrial users, with the objective to set up standard practices to define the quality of CFD simulations and to assess the trustworthiness of the CFD results. The initiative was concerned with the issue of “Quality” and has led to the publication of the first edition of the ERCOFTAC Best Practice Guidelines (BPG), Casey and Wintergerste^[2] (for details see the section “publications” on the ERCOFTAC Website—www.epfl.imhef/ERCOFTAC). The BPG provides generic advice on how to perform quality CFD calculations, and this action identified also the objectives for the follow-up steps and the need to collect CFD and experimental data in a more systematic and quality controlled way, and to set the basis for a consistent KB in support of CFD guidance and validation, Hutton and Casey (2001). As a followup initiative, QNET-CFD set its objective towards the production of a set of Application Procedures (AP) and associated database of simulations and experimental data which will allow industrial practitioners of CFD in specific application areas to interpret results from a position of trust. Thus will comprise a compilation of CFD calculations and tests data in a database for a wide range of test cas-

es chosen for their industrial interest, and carried out according to the BPG. For each test case, the performance of various turbulence and associated models will be analysed, bounds quantified, and advice offered on which calculated flow parameters can or cannot be trusted. This ambitious objective guided the 43 research and industrial groups, including the four major CFD software vendors, part of the QNET-CFD partnership. The initial goals were formulated as follows:

- To assemble, structure and collate existing knowledge on the industrial application of CFD and to make these available to European industry
- To improve the quality of the industrial application of CFD
- To improve the level of trust that can be placed in industrial CFD calculations by assembling, structuring and collating existing knowledge under the form of Best Practice Advices
- To establish a shared database of computational and experimental results to support industrial applications
- To provide a regular state-of-the-art review on quality and trust
- To promote technology transfer between industries through work-shops, regular meetings and electronic communication

The QNET-CFD activity was organised around 6 Thematic Areas (TA) aligned with the following industrial sectors:

- TA1: External Aerodynamics
- TA2: Combustion & Heat Transfer
- TA3: Chemical & Process, Thermal Hydraulics and Nuclear Safety
- TA4: Civil Construction & HVAC
- TA5: Environment
- TA6: Turbomachinery Internal Flows

Procedures were established towards the set objectives, based on a hierarchy of test cases classified as Application Challenges (AC) and Underlying Flow Regimes (UFR). An AC is defined as

- An industrial test case by which the competency of CFD for the sector is judged
- Key design or assessment parameters are de-

defined

- Key design or assessment parameters are measured

- CFD calculations are available

An UFR is defined as:

- A generic flow configuration or process which captures a key element of the fluid physics associated with an AC

- The set of UFR-s connected to a given AC represent the important mechanisms which control the fluid dynamic behavior of the AC

- A given UFR is likely to be associated with more than one, perhaps many ACs

- It is expected that detailed sets of measurements & well resolved CFD calculations are available for each UFR

A particular attention has been given to the Quality Procedures allowing

- To filter the AC's and the UFR's against quality requirements, assessing the level of reliability of the experimental as well as the related CFD data

- Identify the best and most representative UFRs

- Documentation of data/calculations connected to UFR's

Each UFR can be attributed to several AC's, and contains experimental data and a variety of CFD simulations, from which Best Practice Advice (BPA) guidelines are derived. From the collection of BPA's of all the UFR's associated to an AC, a BPA for the AC is to be established.

The assembled, structured and collated knowledge acquired from the AC's and UFR's is made available in the Knowledge Base (KB), as shown in Fig. 1.

1.1 Quality control procedures

All entries into the KB have undergone rigorous quality checks against defined standards. To streamline the process of incorporating the information contributed to the KB, templates were created to provide guidance on what should be included and the minimum level of detail. The objective was to ensure a common format for the presentation of the

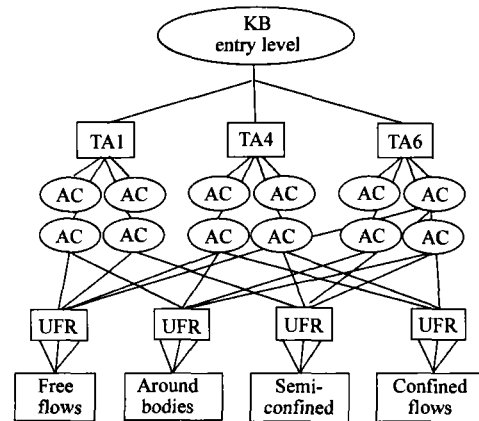


Fig. 1 KB structure

data and a common level of information. All the AC, UFR and associated BPA were mutually peer reviewed before being accepted for inclusion into the KB. To standardise the process 'Quality checklists' were created, which were used to record the outcome of the review of each of the KB components.

2 KB Design and Development

The design and development of the KB were set out to structure and present the information in a format that would: i) be accessible *via* the Internet; ii) have user-friendly structure; iii) support the interpretation of existing knowledge; iv) provide BPA; v) promote transfer knowledge across industry sectors; vi) help identify gaps in current knowledge; vii) be expandable and grow to include new knowledge.

2.1 Structure and content of the KB

The KB is structured around the six Thematic Areas (TAs) and the four Underlying Flow Categories. The AC are associated with a single TA or industry sector. The UFR are linked to AC across the TA. This is an important feature of the KB, with which transfer of knowledge between industry sectors is achieved.

BPA on how to carry out CFD simulations is provided for each of the AC and UFR. The advice given at each level represents a synthesis of all related information; the advice specific to each AC takes into account the advice given in each of the

related UFR.

Reviews on the State-of-the-Art application of CFD are also provided at the Thematic Area level.

The KB currently contains more than 40 AC, more than 40 UFR, records of the quality reviews, BPA for each AC and UFR, 6 State-of-the-Art Reviews (one for each TA) and all the Templates and Quality Procedures used in the course of the QNET-CFD development.

Users can navigate through the entire KB using an Internet browser. The entry level page of the KB is shown in the Fig.2.

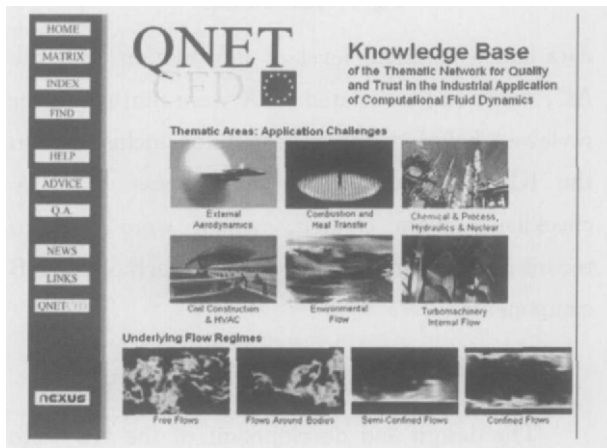


Fig.2 The entry level of the QNET-CFD KB

Hyperlinks provide cross-linkages between the Industrial sectors, AC and UFR. A navigation bar on the left of the screen helps users to keep track of their location within the KB. Users may go directly to any part of the KB via contents lists (Index), summary matrix tables (Matrix) and keyword search facilities (Find). The entry level is shown in Fig.2.

2.2 The application challenges

The AC's are attached to the 6 thematic areas and cover a wide range of test cases and flow configurations.

(1) For TA1: External aerodynamics

- Aero-acoustic cavity
- RAE M2155 Wing
- RAE 2822 Airfoil
- Channel flow with wall injection
- Ahmed body
- L1T2 3 element airfoil
- AS28G Wing-Body-Pylon-Nacelle

• Yawing and Spinning Projectile

(2) For TA2: Combustion & heat transfer

- Bluff body burner for CH₄-HE turbulent combustion
- Thermo-capillary flow in cylindrical liquid bridge
- Gas burner controlled by variable density and/or counter flow
- Generic bluff body combustion
- Airflow cyclic variations in IC engines
- The confined TECFLAM swirling natural gas burner

• Confined double annular jet

(3) For TA3: Chemical & process, thermal hydraulics and nuclear safety

- Buoyancy-opposed wall jet
- Induced flow in a T-junction
- Cyclone separator
- Buoyant gas air-mixing
- Gas release from high pressure pipelines

(4) For TA4: Civil construction & HVAC

- Wind environment around an airport terminal building (Built environment, external)
- Flow and sediment transport in a stretch of the river Elbe (Hydraulics)
- Tunnel fire (Transport and Infrastructure, Tunnels)
- Aerodynamic analysis of the great belt bridge (Built environment, external)
- Coastal flow and sediment transport
- Air flows in an open plan air conditioned office (Built environment, internal)

(5) For TA5: Environment

- Flow and dispersion in the presence of an L-shaped building
- Dense gas release over flat terrain with and without obstruction
- Urban scale problems
- Mesoscale wind flow and dispersion
- Boundary layer flow over isolated hills and valleys

(6) For TA6: Turbomachinery internal flows

- Low-speed centrifugal compressor
- Annular compressor cascade without clear-

ance

- Pump turbine
- Annular compressor cascade with tip clearance

ance

- Gas Turbine nozzle cascade
- Draft tube
- High speed centrifugal compressor
- High speed axial compressor
- Axial compressor cascade
- Turbine cascade with cooling holes
- Steam turbine rotor cascade

2.3 The Underlying Flow Regime (UFR) test cases

The UFR's are subdivided in four classes, covering a wide range of basic flow configurations.

UFR1: Free flows

UFR2: Flow around bodies

UFR3: Semi-confined flows

UFR4: Confined flow

(1) UFR1: Free flows

- Underexpanded jet
- Blade tip and tip clearance vortex flow
- Annular coaxial jets, flow and mixing
- Jet in a cross flow

(2) UFR2: Flow around bodies

- Flow behind a blunt trailing edge
- Flow past cylinder
- Flow around oscillating airfoil
- Flow around (airfoils and) blades (subsonic)
- Flow around airfoils (and blades) A-airfoil

($Ma = 0.15$, $Re/m = 2 \times 10^6$)

- Flow around (airfoils and) blades (transonic)

ic)

- 3D flow around blades
- Rotor/stator interaction

(3) UFR3: Semi-confined flows

• Boundary layer interacting with wakes under adverse pressure gradient-NLR 7301 high lift configuration

• Atmospheric boundary layer with rough wall (mesoscale)

- 2D Boundary layers with pressure gradients
- Laminar-turbulent boundary layer transition

• Shock/boundary-layer interaction (on air-planes)

• Natural and mixed convection boundary layers on vertical heated walls (A)

• Natural and mixed convection boundary layers on vertical heated walls (B)

• 3D boundary layers under various pressure gradients, including severe adverse pressure gradient causing separation

- Impinging jet
- The plane wall jet
- Pipe expansion (with heat transfer)
- Stagnation point flow
- Flow over an isolated hill (without dispersion)

• Flow over surface-mounted cube/rectangular obstacles

• 2D flow over backward facing step

• Wave-driven flow in a basin

• Bypass transition on a flat plate

(4) UFR4: Confined flows

• Secondary flow in rotating and non-rotating channels

• Confined coaxial swirling jets

• Pipe flow-rotating

• Flow in a curved rectangular duct-non rotating

• Curved passage flow

• Swirling diffuser flow

• Developing channel flow with mass injection through wall

• Orifice/deflector flow

• Confined buoyant plume

• Natural convection in simple closed cavity

• Simple room flow

• Compression of vortex in cavity

• Flow in pipes with sudden contraction

3 Examples of Best Practice Advice

As an illustration of the results accumulated in the KB, we focus on the outcome of TAI, related to external aerodynamics and some representative AC's.

3.1 AC1-02 RAE M2155 wing

The RAE M2155 wing has been the subject of many numerical simulations and was used to validate and assess turbulence models in several EU funded projects. The wing is swept, of low-aspect ratio, and has the plan form shown in Fig. 3. Experiments were performed at the DERA 8ft \times 6ft transonic wind tunnel in the Mach number range 0.6-0.87 and at a Reynolds number (based on the geometric mean chord) of 4×10^6 .

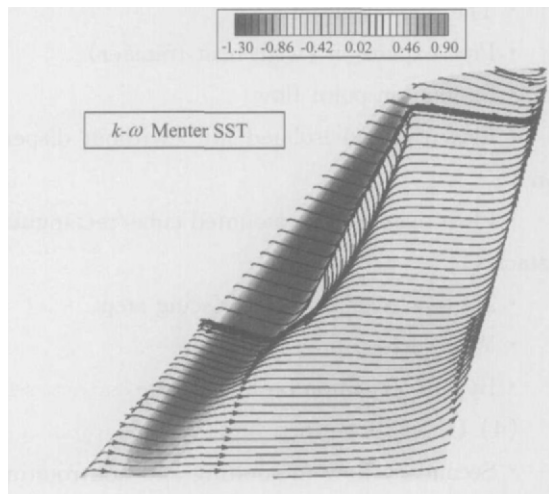


Fig. 3 Pressure contours and skin friction lines RAE M2155 wing

The wing presents a complex flow field with three-dimensional separations and triple shock wave structures. The boundary layers are subject to strong adverse pressure gradients (the trailing edges are heavily loaded), a regime which is difficult for numerical methods but of great importance in wing design. Case 2, with a Mach number of 0.806 and an angle of attack of 2.5° , is the most severe, and has been used for QNET-CFD. Application uncertainties for this case are the influence of the tunnel walls and the interaction between the boundary layers on the tunnel wall and the wing. For this reason, CFD simulations should include the wind tunnel walls.

The following Underlying Flow Regimes are associated with this application challenge:

UFR3-03: Boundary layers with pressure gradients

UFR3-05: Shock-boundary layer interaction

UFR3-08: 3D Boundary layers subject to strong adverse pressure gradient causing separation

The Best Practice Advice particular to this test case are:

Use at least 10 grid points in the streamwise direction across the shock.

Fix the transition locations in the same way as in experiments.

Use turbulence models with non-linear constitutive relation or the Menter SST $k-\omega$ model to predict the shock location, the pressure recovery behind the shocks and velocities in zones with flow separation.

3.2 AC1-05 Ahmed body

The shape of the Ahmed body contains all the important features of real road vehicles; a main body, followed by a fully separated region. Prediction of separated flows is one of the more difficult tasks of CFD. The parametric variation of the angle of the rear part (slant angle) of the Ahmed body permits the study of various configurations relevant to real car characteristics, from massively separated “simple” wakes to very complex 3D wake structures. The reproduction of the complex 3D wake is very challenging for CFD, as well as the transition from one behavior to another. Two experimental data bases exist for the Ahmed body. The first data base contains drag values for different values of the rear angle. These drag values are closely linked to the structure of the wake. The second experimental data base provides very detailed results, including turbulent quantities that are useful for a detailed analysis of turbulence models.

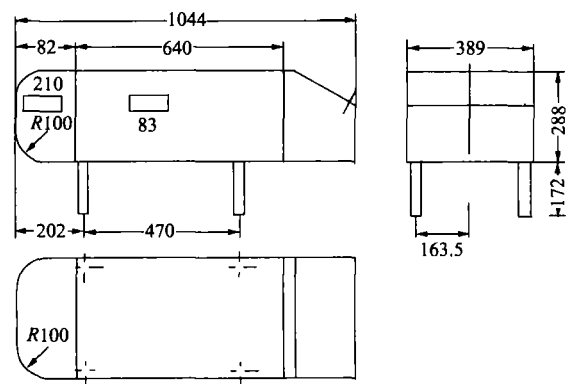


Fig. 4 Shape of Ahmed body

Uncertainties in experimental results are the influence of the stilts, which affect the flow under the body and the wake, and the use of an experimental facility with a 3/4 open test section.

The key physics in this complex flow is connected to the sensitivity of the drag coefficient with the slant angle. The contributions of the different components of the drag have different trends when the slant angle changes. The topology of the flow is crucial for the correct reproduction of the drag coefficient: in particular, the drag crisis around 25°-30° corresponds to a transition of the wake structure from a massively separated, quasi-2D structure to a complex, 3D structure. The component responsible for the drag crisis is the pressure drag due to the slant part, which jumps from 35% of total drag at 35° to 55% at 25°. The drag crisis corresponds to a dramatic change in the structure of the wake, since in the low-drag configuration, the wake is massively-separated, quasi-toroidal. In the highdrag configuration, the wake has a complex, 3D structure: in the central region of the slant part (close to the symmetry plane) experiments show a small separation bubble, with a reattachment on the slant part. This bubble strongly interacts with the highly energetic corner vortices. Other complex phenomena are present (interaction with the underside flow, with side boundary layers, large-scale flapping in the spanwise direction, *etc.*), but they are not well understood yet.

The available experience led to the following observations:

(1) Low-drag configurations

All the turbulence models used in the CFD studies give a correct wake structure and C_d trend when varying the angle for low-drag configurations. However, using low- Re models gives a better boundary layer prediction on the slant part. None of the models give the correct quantitative prediction of the pressure distribution on the slant part and vertical base, and, therefore, of the drag. For qualitative predictions in the low-drag configuration, simple eddy-viscosity models with wall functions are sufficient, but quantitative predic-

tions cannot be trusted, what ever the model.

(2) High-drag configurations

High Reynolds number models (k - ϵ , RSM) with wall functions must be avoided, because they generally do not predict separation at all, and always fail predicting correct profiles above the slant part.

Low- Re eddy-viscosity models predict separation provided they are free from the usual stagnation point anomaly (over-prediction of turbulence production: this is the case for the k - ω /SST model, for non-linear/algebraic k - ϵ and k - ω models and the rescaled V2F model. These models predict massive separation, far from experiments.

Low Reynolds stress models seems to be able to reproduce (too late) reattachment on the slant part and the qualitatively correct wake structure. However, this needs to be confirmed by further studies.

LES is clearly able to reproduce the correct structure of the wake. However, using resolution down to the viscous sublayer is clearly unaffordable for the time being and the use of wall functions does not allow the correct reproduction of the boundary layer above the slant part.

The Best Practice Advice for the turbulence modelling depends strongly on the slant angle. A distinction is made between low drag and high drag configurations. For low drag configurations (slant angle 35°), simple eddy viscosity models with wall functions are sufficient for qualitative predictions (overall evolution of the drag with the slant angle and the wake structure). Quantitative predictions of the pressure distribution and the drag can not be trusted using any turbulence model used. For high drag configurations (slant angle of 25°), only very refined turbulence models give the correct wake structure (Low Reynolds number second moment closure or LES). Turbulence models employing wall functions must be avoided, as well as models leading to a stagnation point anomaly.

Since accounting for the near-wall region (low- Re RSM) and the large-scale unsteadiness (LES) have beneficial effects, the potential of ac-

counting for both must be investigated with RANS/LES zonal coupling, RANS/LES hybrid models, DES methods.

3.3 AC1-08 L1T2 multi element airfoil

This application challenge is focused on one of the 2D high lift configurations (the L1T2 test case). The L1T2 case is a 3 element aerofoil consisting of a main element, a slat forward of the main element (deflection angle 25°), and a Fowler flap aft of the main element (deflection angle 20°). See Fig. 5. Measurements were made at two incidences, one at a low angle of attack and one close to maximum lift. The main flow physics is characterized by strong interactions between the turbulent boundary layers and wakes of the slat/wing/flap elements. The interaction between a wake and a downstream boundary layer can lead to boundary layer thickening and separated flow. The flow is considered to be two-dimensional. The L1T2 configuration was tested at a Mach number of 0.197, using a Reynolds number of 3.52×10^6 (based on retracted chord) and at angles of incidence (corrected) of 4.01° and 20.18° .

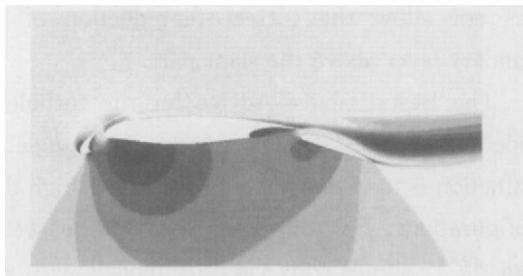


Fig. 5 Mach number contours L1T2 multi element airfoil

The relevant UFRs are UFR3-01 (Boundary Layer-Wake Interaction NLR 7301), UFR3-03 (2D Boundary Layers with pressure gradients) and UFR3-04 (Laminar turbulence).

Application uncertainties for this test case concern the position location, which is not specified and may have a significant influence on the overall forces, in particular at high incidence angle, and the resolution of the wake.

Best Practice Advice particular for this case are:

- If a far-field circulation correction method is used at the far-field boundary, ensure that the far-

field boundary is at least 15 chord lengths away. If not, ensure that the far-field boundary is at least 50 chord lengths from the body.

- Use the full, compressible, Reynolds Averaged Navier-Stokes formulation.

- If an accurate prediction of the pressures on the lifting surfaces (and so lift coefficient) is required. USE the $k-\omega$ turbulence model.

- It is not possible to give advice on which turbulence model to use for the accurate prediction of boundary layer profiles and wakes.

4 Best Practice Advice Common to All Application Challenges

- Use at least a second order accurate scheme with as little as numerical dissipation possible.

- For low Reynolds number turbulence models, use a y^+ of $O(1)$ for the first layer of cells, with 5-10 grid points up to $y^+ = 20$ from the wall, and in total 30-60 points across the boundary layer.

- For turbulence models using a wall function approach, use a mesh with wall adjacent heights $30 < y^+ < 100$.

5 Conclusion

The QNET-CFD KB is a unique resource. It embodies the knowledge contributed by a large number of experienced CFD users, covering several industrial sectors.

It is hoped that the well-defined process developed for documenting and reviewing CFD knowledge will encourage the inclusion of new information, expanding both the existing thematic area content and inspiring the development of new thematic areas. Indeed, it is envisaged that in the future it will be widely adopted as the primary mechanism for the publication and dissemination of CFD research work.

During the period the QNET-CFD Network has been in place the KB has remained confidential to the Network members and associated members who have contributed Application Challenges or Underlying Flow Regimes.

However, after the end of QNET-CFD in July

2004 the aim is to make the KB widely available, and to ensure that its content will expand and be updated with new contributions. This is now being undertaken by ERCOFTAC.

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